Part 6: MCMC and Bayesian Modeling Part II

January 11, 2021

If you recall the post on January 4, 2021 discussing the basics of Bayesian modeling using Gibbs and Hamiltonian-Monte Carlo Sampling (HMC), both use *Bayes Rule* with a prior $\pi(\theta)$ over the parameter and a likelihood $p(x|\theta)$:

$$Pr(\theta|x) =\propto \pi(\theta)p(x|\theta) \tag{1}$$

Here we will go over some fun examples of using this simple rule to solve a variety of problems!

1 A Probit Model for Death Probability

Let's say we have a binary classification problem $y \in [1, 0]$ where we have indicator variables $X = [1, x_{age}, x_{gender}]$ (1 is for a bias/intercept) where $y_i = 1$ indicates a person died and $x_{gender} = 1$ indicates a person was male (in the example I took this from it's the *Donner Party* survival statistics). First we need a mathematical model. We shall use the probit model where Φ is the standard normal probability density function (which will utilize a linear model $\beta^T x_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2}$):

$$Pr(y_i = 1|x_i) = \Phi(\beta^T x_i) \tag{2}$$

It may be obvious to smart people, of which I am not, but the likelihood function for this model is as follows:

$$L(x_i, X, Y, \beta) = \Pi_i^N \Phi(\beta^T x_i)^{y_i}(1 - \Phi(\beta^T x_i))^{1-y_i} \tag{3}$$

We can use a simple non-regularizing prior:

$$Pr(\beta) = 1 \tag{4}$$

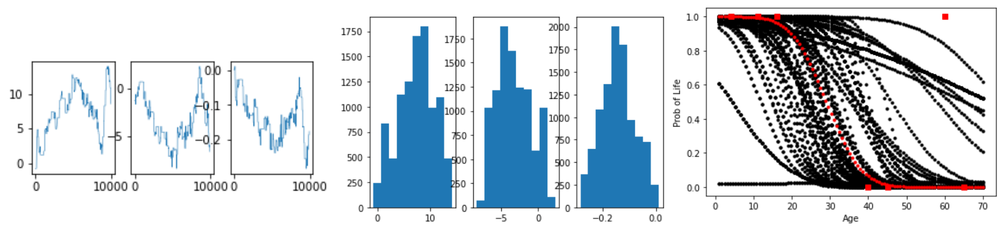
I will write out the full HMC algorithm for everyone here (also check the code attached):

Data: $p(\beta)$ Posterior Equations
Result: $B \sim Pr(\beta)$ Posterior Sample
Initialize θ;
for $k = 1 : K$ *Samples* **do**

$\beta_p \sim N(\beta, I)$;
$p(\beta) = 1 \times L(X, Y, \beta)$;
$p(\beta_p) = 1 \times L(X, Y, \beta_p)$;
$q(\beta|\theta_p) = N(\beta|\mu = \beta_p, I)$;
$q(\beta_p|\beta) = N(\beta_p|\mu = \beta, I)$;
$\alpha = min\{1, \dfrac{p(\beta_p)q(\beta|\beta_p)}{p(\beta)q(\beta_p|\beta)}\}$;
$Pr(\beta = \beta_p = B_k) = \alpha$;

end

Algorithm 1: Hamiltonian-Monte Carlo Sample



(a) Chains (b) Posterior of β (c) Posterior of $Pr(y = 0|x)$ for Males

Figure 1: Bayesian Probit Model for Survival

Where the parameters for the probit model are $\beta = [\beta_0, \beta_{age}, \beta_{gender}]$. We find from Figure 1(b) that the distribution of the model parameters are $\beta_{age}, \beta_{gender} < 0$. This indicates that being older and a male are correlated with the outcome $Pr(y_i = 1|x_i)$ (death). The theory is that older people are weaker and women have more body-fat / weight than men, so younger people and women were more likely to survive the *Donner Party*.

2 Gaussian Process Model Solved using HMC

Now let's look at the Gaussian process model (GP) from our first official post! Remember the mean $\hat{\mu}$ and standard deviation $\hat{\sigma}^2$ of the model is in the following form:

$$\hat{\mu} = K(x, X)(K(X, X) + \sigma^2 I)^{-1} Y \tag{5}$$

$$\hat{\sigma}^2 = K(x, x) - K(x, X)(K(X, X)^{-1} K(X, x) \tag{6}$$

Where we have a kernel matrix $K(x, x')$ that relates a point x to another point x' (usually through a Euclidean distance metric). If you also recall, the likelihood function is as follows:

$$L(\sigma, \sigma_f, l) = -0.5 Y K_y Y^T - 0.5 log(det(K_y)) - 0.5 n log(2\pi) \tag{7}$$

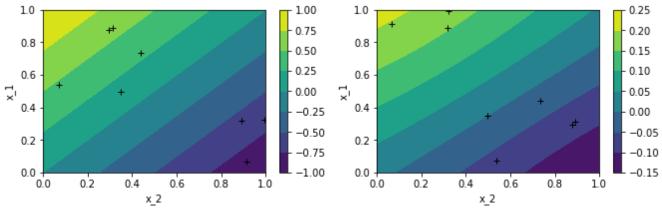
$$K_y = K(X, X) + \sigma^2 I \tag{8}$$

Well, we have a likelihood, all we need is a prior. Let's use the same non-regularizing priors as in Equation (4). Let's train our model on input data X and output data Y using $N = 8$ data points for the test function $f(x_1, x_2) = x_1 - x_2 + U(0, 0.1)$. To be clear, we are "training" using the HMC algorithm detailed in the previous post with the posterior:

$$Pr(\sigma, \sigma_f, l|X, Y) = L(X, Y|\sigma, \sigma_f, l) Pr(\sigma) Pr(\sigma_f) Pr(l)$$

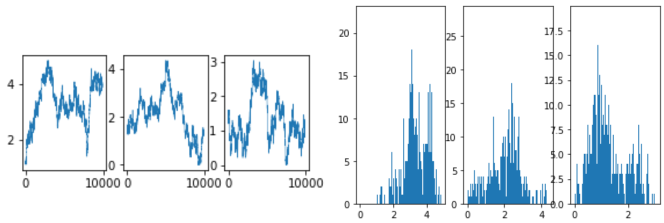
This one was a little harder to solve with an extremely generic HMC algorithm (no fancy tricks that *stan* might use) but using $M = 10^5$ HMC iterations and a proposal distribution of $Pr(\beta_p|\beta) = N(0, 10^{-3} I)$ for all parameters β I was able to get reasonable regression (by shrinking the proposal distribution variance, the Markov Chains are less likely to move in extreme directions). The results in Figure 2 show at least reasonable estimates, which points in the direction that we are on the road to building our own HMC algorithms!

The results for the chains are not perfect. In fact while the distributions may show a clustering around particular means, and the final results for regression aren't terrible, the dynamics of the chains are a different story.



(a) Data (b) GP with HMC Solved θ

Figure 2: GP Test Problem Results



(a) Chains (b) Posterior of θ

Figure 3: HMC Posterior Results

3 Convergence and Output Analysis

The primary means of analysis of convergence (or the stationarity) of the posterior is via the Gelman-Rubin approach. In this approach we calculate the metric:

$$\hat{R} = (\frac{V(B|X)}{W})^{1/2} \tag{9}$$

$$V(B|X) = \frac{K-1}{K}W + \frac{1}{K}b$$

$$b = \frac{K}{M-1}\Sigma_j^M(\hat{B}_{.j} - \hat{B}_{..})^2$$

$$W = \frac{1}{M}\Sigma_j^m s_j^2$$

$$s_j^2 = \frac{1}{K-1}\Sigma_i^K(B_{ij} - \hat{B}_{.j})^2$$

$$\hat{B}_{.j} = \frac{1}{K}\Sigma_i^K B_{ij}$$

$$\hat{B}_{..} = \frac{1}{M}\Sigma_j^M \hat{B}_{.j}$$

Yes I know that's a lot (and it is). So go through the code where I make each of these calculations step by step and see what's going on here. The variable b and W are two measures of variance. For our analysis we break each chain into two chains for a total of M chains. We don't utilize 'burn-in' period in which we ignore the first (usually $0.25K$) few posterior solutions. In our example problem let's use HMC on the GP problem above with $K = 100$ samples, five chains for a total $M = 10$.

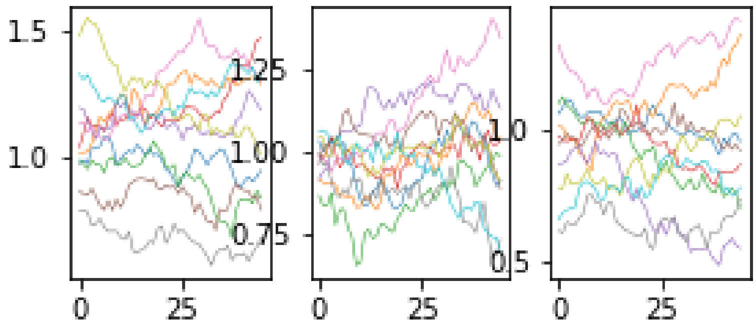


Figure 4: HMC Chains for GP Problem

Notice that the chains are kind of everywhere, but that is all relative. We are really just trying to get a feel for the math and simulation behind MCMC and not spend time doing perfect implementation. I'll just say here (i) we'd want to have a burn-in period, (ii) we'd want a stronger algorithm (such as the powerful NUTS Sampler used in PYMC3) and/or (iii) better use of priors.

Finally we have the solution to the GP problem in $\hat{R}$ (In general you want $1.1 < \hat{R} < 1$):

$$\hat{R} = \begin{pmatrix} 1.4 \\ 1.3 \\ 1.5 \end{pmatrix}$$

Done for today. We will be leaving MCMC for now and next week we'll go over a fun global optimization method: Trust Regions!